

## PATENT ABSTRACTS OF JAPAN

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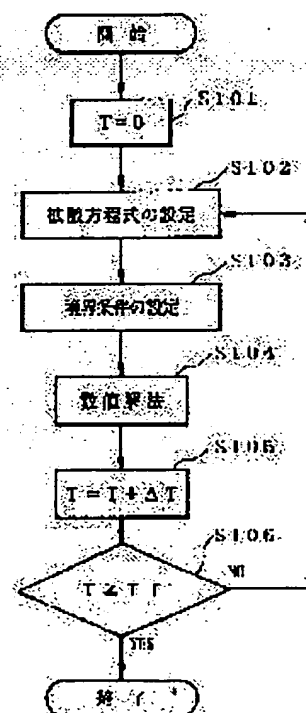
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## (54) SIMULATION METHOD

## (57)Abstract:

PROBLEM TO BE SOLVED: To obtain analysis of high precision in a narrow calculation region by setting the boundary condition of a region for simulation, in such a manner that impurities or point defect move across the boundary of the calculation region.

SOLUTION: Diffusion time  $T$  is set to 0 (S 101). By calculating the diffusion coefficients or the like at a diffusion temperature, a diffusion equation is set (S 102). The boundary of the simulation region, i.e., the boundary condition to a substrate bottom surface is so set, that it is allowed for impurities or point defects to exceed the boundary of the calculation region and move (S 103). After the boundary condition and the diffusion equation are set, analysis of the diffusion equation is obtained by using a numerical analysis method (S 104). Next, the diffusion time  $T$  is increased by  $\Delta T$  (S 105). Whether the value exceeds the total diffusion time  $T_f$  is judged (S 106). When it exceeds  $T_f$ , the loop which starts from the setting of the diffusion equation is again executed.



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CLAIMS

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[Claim(s)]

[Claim 1] The simulation approach characterized by including setting up so that it may permit that an impurity or a point defect moves to the boundary of the field which performs simulation across the boundary of a count field as boundary condition in the approach of performing the impurity or point defect diffusion simulation of a semi-conductor production process.

[Claim 2] Said boundary condition is the simulation approach according to claim 1 characterized by determining the boundary condition of the boundary concerned that the movement magnitude of the impurity which passes through the boundary concerned, or a point defect will become equal to the movement magnitude obtained when it calculates in sufficient large field including the field concerned.

[Claim 3] Said boundary condition is the simulation approach according to claim 1 characterized by determining the boundary condition which an impurity moves across a boundary using the fine multiplier of the impurity profile of the direction [ / near the boundary ] of a boundary normal.

[Claim 4] Said boundary condition is the simulation approach according to claim 1 characterized by determining the boundary condition which an impurity or a point defect moves across a boundary by approximating the impurity or point defect profile of the direction of a boundary normal with a gauss function. [ / near the boundary ]

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DETAILED DESCRIPTION

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## [Detailed Description of the Invention]

[0001]

[Field of the Invention] Especially this invention relates to the technique used for the impurity or point defect diffusion simulation of a semi-conductor production process about the simulation approach.

[0002]

[Description of the Prior Art] With high integration of an integrated circuit, the number of production processes increases and the process itself is complicated. For this reason, the count of a prototype increases and development cost is going up. In order to cope with such a situation, prototype conditions are beforehand narrowed down using a simulator, the count of a prototype is reduced, and efforts to shorten a prototype period are made. For example, in the case of the process simulation, simulation, such as an ion implantation and oxidation / diffusion process, was performed using the process simulator, a component configuration and impurity distribution were predicted, and the process conditions of a prototype were narrowed down so that the result might become a desired value.

[0003] The process simulation is holding the trouble that the amount of memory which computation time starts and needs also increases, if simulation of the large component field is carried out. Impurity diffusion simulation occupies most of computation time which a process simulation takes, and amounts of memory. Therefore, if the computation time and the amount of memory which the impurity diffusion simulation of a large field takes are reducible, it will become possible to perform a process simulation efficiently.

[0004] What is necessary is just to limit a simulation field to a required part, in order to perform impurity diffusion simulation in the small amount of memory at high speed. However, in the conventional impurity diffusion simulation, since reflective mold boundary condition was used for the boundary of a count field, when the count field was narrow, the impurity was shut up in the boundary, and there was a problem that the precision of a solution fell. Since it is easy, 1-dimensional simulation of a well formation process is made into an example, and this is explained.

[0005] Drawing 3 is a graph at the time of carrying out the 100keV(s) and  $3 \times 10^{13}/\text{cm}^2$  ion implantation of the boron of doses to a silicon substrate. The axis of abscissa of this graph shows the depth from a silicon substrate surface, and an axis of ordinate shows the concentration of boron. The diagrammatic dotted line A expresses the profile immediately after an ion implantation. Moreover, in order to calculate the profile of the boron when being spread at 1200 degrees C for 4 hours with a sufficient precision, a broken line B shows the result calculated from a substrate front face to a depth of 8 micrometers.

[0006] Generally, since many of component properties should just have a profile with a depth of 2 micrometers in calculating the threshold of MOSFET from a substrate front face, it calculates a count field by limiting it to this field from the reasons of shortening of the processing time etc. in many cases. An alternate long and short dash line C shows the profile in this case. In both cases, the boundary condition at the base of a substrate is using the reflective mold. If a count field is narrowed from this drawing, the precision of a solution is getting very worse so that clearly from the result of an alternate long and short dash line C.

[0007]

[Problem(s) to be Solved by the Invention] Thus, when reflective mold boundary condition was used for the boundary of an impurity diffusion simulation field, and the count field was narrowed, there was a

problem that the precision of a solution fell. In order that precision might improve simulation, when the simulation field was made large, on the other hand, the required amount of memory increased and there was a problem that computation time became long. 8

[0008] This invention is made in view of the above-mentioned situation, and the place made into the purpose is to offer the simulation approach that a highly precise solution can be acquired, even if it is a narrow count field.

[0009]

[Means for Solving the Problem] In order to attain the above-mentioned purpose, invention of claim 1 is characterized by including setting up so that it may permit that an impurity or a point defect moves to the boundary of the field which performs simulation across the boundary of a count field as boundary condition in the approach of performing the impurity or point defect diffusion simulation of a semiconductor production process.

[0010] Invention of claim 2 is characterized by the boundary condition in said claim 1 determining that the boundary condition of the boundary concerned will become equal to the movement magnitude obtained when it calculates in sufficient large field in which the movement magnitude of the impurity which passes through the boundary concerned, or a point defect includes the field concerned.

[0011] It is characterized by invention of claim 3 determining the boundary condition to which an impurity moves the boundary condition in said claim 1 across a boundary using the fine multiplier of the impurity profile of the direction [ / near the boundary ] of a boundary normal.

[0012] It is characterized by invention of claim 4 determining the boundary condition which an impurity or a point defect moves across a boundary when the boundary condition in said claim 1 approximates the impurity or point defect profile of the direction of a boundary normal with a gauss function. [ / near the boundary ]

[0013]

[Embodiment of the Invention] Hereafter, the operation gestalt of the simulation approach concerning this invention is explained to a detail, referring to a drawing. In the following operation gestalten, in order to simplify explanation, it considers as the 1-dimensional impurity diffusion simulation in a silicon substrate.

[0014] In the simulation approach explained with the following operation gestalten, the usual computer system equipped with output units, such as CPU for performing various processings, input devices, such as a keyboard, a mouse, a light pen, or flexible disk equipment, external storage, such as a memory apparatus and a disk unit, and a display unit, printer equipment, etc. is used. In addition, said CPU possesses the operation part which performs processing of each step explained below etc., and the primary storage which memorizes an instruction of said processing.

[0015] Gestalt drawing 1 of the 1st operation is a flow chart which shows processing actuation of the impurity diffusion simulation of this operation gestalt. Initiation of diffusion simulation sets the diffusion time of day T to 0 first (step S101). And the diffusion coefficient in diffusion temperature, a segregation coefficient, etc. are calculated, and a diffusion equation is set up (step S102).

[0016] Next, boundary condition is set up on the boundary of a simulation field, i.e., this example, as follows to a substrate base (step S103).

[0017]  $F = -D$  and  $\frac{dC}{dx}$  -- here, D is the diffusion coefficient of an impurity and C is high impurity concentration. This boundary condition means that an impurity flows out of a substrate base outside a simulation field by Flux F. The conventional approach had set up reflective mold conditions ( $F = 0$ ) as boundary condition here. For this reason, the impurity distribution which should spread by diffusion will be shut up for the reflective mold boundary condition set as the base, and concentration becomes high unusually. Although this problem was avoidable when setting up the simulation field sufficiently widely, the problem that computation time became long had arisen.

[0018] Thus, after setting up a diffusion equation and boundary condition, the solution to is calculated using a numerical solution (step S104). Next, the increment of the diffusion time of day T in  $\Delta T$  is done (step S105), if it judges and (step S106) is not over whether the value is over all the diffusion time  $T_f$ , the loop formation which begins from a setup of the diffusion equation of step S102 is executed again, otherwise, count is ended.

[0019] Next, single diffusion simulation of the boron in a silicon substrate is made into an example, and

the effectiveness of this invention is explained. Drawing 2 is 100keV(s) and  $3 \times 10^{13}/\text{cm}^2$  of doses about boron to a silicon substrate. It is a graph at the time of carrying out an ion implantation. The axis of abscissa of this graph shows the depth from a silicon substrate surface, and an axis of ordinate shows the concentration of boron. In order to simplify explanation, the impurity evaporation from a substrate front face was calculated as what is not. Here, it is spread at 1200 degrees C for 4 hours, and the result of having taken the sufficiently deep depth of a substrate with 8 micrometers, and having calculated it with a sufficient precision is shown in a broken line B. Moreover, an alternate long and short dash line C is the result of restricting the depth of a substrate to 2 micrometers and calculating using the conventional approach. By the conventional approach, since reflective mold boundary condition is used as boundary condition at the base of a substrate, boron will be shut up in a count field and has overestimated boron concentration remarkably. A continuous line shows the result which restricted the depth of a substrate to 2 micrometers and was calculated on the other hand using this invention.

[0020] The result depended on the simulation approach concerning this invention is shown in a thick wire D. Since the boundary condition of a simulation boundary was appropriately given like illustration, in spite of having restricted the simulation field to 2 micrometers, it is very well in agreement with the result (broken line B) calculated with a sufficient precision in the sufficiently large field. The impurity distribution near a substrate front face influences a component property greatly. Like drawing 2, since this invention calculates the impurity distribution near a substrate front face with a sufficient precision, the component property that precision is high can be acquired.

[0021] Thus, if this invention is used, simulation can be performed, without losing most precision, even if it narrows a simulation field. Although simulation fields were reduced to the quadrant in this example, it cannot be overemphasized that comparable reduction also of the amount of memory and computation time required for simulation is carried out. Thus, a process simulation can be performed at a high speed in the amount of memory smaller than before by using this invention.

[0022] In addition, although this operation gestalt explained using 1-dimensional simulation in order to simplify explanation, it is clear that this invention is applicable to two-dimensional and three-dimension simulation. It is clear that the amount of memory and the reduction effectiveness of computation time are especially remarkable in two-dimensional and three-dimension simulation.

[0023] What is necessary is just to set up boundary condition with the operation gestalt of the gestalt 1st of the 2nd operation, so that the solution near the solution calculated in the larger field may be acquired although boundary condition was calculated using the differential of impurity distribution by setup of the boundary condition of step S103. Therefore, it sets in this operation gestalt and, in the case of 1-dimensional simulation, is the profile of the direction of a boundary normal of the impurity distribution near the boundary, for example Gauss function  $a \cdot \exp[-b(x-x_0)^2]$

It comes out and approximates.  $x$  expresses the depth from a substrate front face here, and it is  $a$ ,  $b$ , and  $x_0$ . It is a constant. A gauss function becomes a solution to, when a diffusion coefficient is a constant as known well. Therefore, the impurity distribution near the base of a simulation field can be approximated with a sufficient precision with a gauss function. And the flux in a boundary is calculated noting that this gauss function is prolonged outside the field across the simulation boundary, and this value is used as boundary condition. Thus, since numerical differentiation will not be used like the above-mentioned operation gestalt if boundary condition is calculated, count which was not dependent on mesh spacing etc. and was stabilized can be performed. Consequently, a more accurate simulation result than the conventional approach is obtained.

[0024] Although the operation gestalt of the gestalt above of the 3rd operation explained diffusion of the impurity in a silicon substrate, it is also applicable to the diffusion simulation of a point defect and an impurity. Since impurity diffusion is influenced of a point defect, it can describe impurity diffusion with a precision more sufficient [ the diffusion equation which adopted the point defect ] than an impurity independent diffusion equation.

[0025] however, since the diffusion rate was alike and quicker than the impurity, the point defect needed to make the simulation field large very much, when the conventional approach was used. For example, in a substrate front face to a depth of about 10 micrometers, although a count field is good, when a point defect is adopted, it is [ about 100 micrometers of depth numbers ] needed [ with the process simulation of the usual MOSFET / field ]. For this reason, computation time was very long when a lot of memory

was needed, in order to carry out simulation which took in point defect diffusion.

[0026] However, a count field required for impurity independent diffusion is set up, for example, and boundary condition is applied to a point defect by the approach used to the impurity with the 1st operation gestalt. If it does in this way, also in a narrow field comparable as the case where only impurity diffusion is dealt with, simulation becomes possible and the amount of memory requirements and computation time can be reduced sharply.

[0027] If the operation gestalt of these simulation approach is used as explained above, the process simulation of a semiconductor device can be limited to a required field, and can be performed.

Therefore, it becomes possible in the amount of memory smaller than before to perform simulation at a high speed. Moreover, although there was a case where the precision of the count result obtained when the simulation field was narrow got very bad, by the conventional approach, since the fall of count precision is controlled even if a simulation field is narrow, if this invention is used, possibility of being confused by the inaccurate count result can be reduced.

[0028] If boundary condition is calculated using the differential of the impurity profile of the direction of a boundary normal as the 1st operation gestalt explained, the effectiveness of this invention is realizable only by repairing a little conventional program. Moreover, it is so short that computation time required for count of boundary condition can almost be disregarded if it is compared with the computation time which simulation takes.

[0029] Moreover, as the 2nd operation gestalt explained, boundary condition approximates the direction profile of a boundary normal of the impurity distribution near the boundary with a gauss function, it calculates the flux in a boundary, assuming that this function is prolonged outside a boundary, and sets up boundary condition using this. Since boundary condition can be set up without using numerical differentiation if it does in this way, the boundary condition for which it is hard to depend on the mesh used for numerical calculation can be set up.

[0030] Furthermore, as the 3rd operation gestalt explained, it is applicable not only to impurity diffusion but the diffusion simulation of a point defect and an impurity. the diffusion rate of an impurity boiled the point defect markedly, and since it was quick, when the conventional approach was used, it needed to make the simulation field large very much. For this reason, in order to carry out simulation which took in point defect diffusion, a lot of memory was needed, and computation time was very long. However, if this invention is applied, also in a narrow field, simulation becomes possible and the amount of memory requirements and computation time can be reduced sharply.

[0031] In addition, the program for realizing the simulation approach mentioned above can be saved at a record medium. This record medium can be made to be able to read according to a computer system, and the simulation approach mentioned above while executing said program and controlling the computer can be realized. Here, with said record medium, equipments which can record a program, such as a memory apparatus, a magnetic disk drive, and an optical disk unit, are contained.

[0032]

[Effect of the Invention] As explained above, in case simulation in a semi-conductor production process, such as impurity diffusion and a point defect, is performed according to the simulation approach concerning this invention, even if it is a narrow count field, a highly precise solution can be acquired.

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TECHNICAL FIELD

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PRIOR ART

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[0003] The process simulation is holding the trouble that the amount of memory which computation time starts and needs also increases, if simulation of the large component field is carried out. Impurity diffusion simulation occupies most of computation time which a process simulation takes, and amounts of memory. Therefore, if the computation time and the amount of memory which the impurity diffusion simulation of a large field takes are reducible, it will become possible to perform a process simulation efficiently.

[0004] What is necessary is just to limit a simulation field to a required part, in order to perform impurity diffusion simulation in the small amount of memory at high speed. However, in the conventional impurity diffusion simulation, since reflective mold boundary condition was used for the boundary of a count field, when the count field was narrow, the impurity was shut up in the boundary, and there was a problem that the precision of a solution fell. Since it is easy, 1-dimensional simulation of a well formation process is made into an example, and this is explained.

[0005] Drawing 3 is a graph at the time of carrying out the 100keV(s) and  $3 \times 10^{13}/\text{cm}^2$  ion implantation of the boron of doses to a silicon substrate. The axis of abscissa of this graph shows the depth from a silicon substrate surface, and an axis of ordinate shows the concentration of boron. The diagrammatic dotted line A expresses the profile immediately after an ion implantation. Moreover, in order to calculate the profile of the boron when being spread at 1200 degrees C for 4 hours with a sufficient precision, a broken line B shows the result calculated from a substrate front face to a depth of 8 micrometers.

[0006] Generally, since many of component properties should just have a profile with a depth of 2 micrometers in calculating the threshold of MOSFET from a substrate front face, it calculates a count field by limiting it to this field from the reasons of shortening of the processing time etc. in many cases. An alternate long and short dash line C shows the profile in this case. In both cases, the boundary condition at the base of a substrate is using the reflective mold. If a count field is narrowed from this drawing, the precision of a solution is getting very worse so that clearly from the result of an alternate long and short dash line C.

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EFFECT OF THE INVENTION

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[Effect of the Invention] As explained above, in case simulation in a semi-conductor production process, such as impurity diffusion and a point defect, is performed according to the simulation approach concerning this invention, even if it is a narrow count field, a highly precise solution can be acquired.

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TECHNICAL PROBLEM

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[Problem(s) to be Solved by the Invention] Thus, when reflective mold boundary condition was used for the boundary of an impurity diffusion simulation field, and the count field was narrowed, there was a problem that the precision of a solution fell. In order that precision might improve simulation, when the simulation field was made large on the other hand, the required amount of memory increased and there was a problem that computation time became long.

[0008] This invention is made in view of the above-mentioned situation, and the place made into the purpose is to offer the simulation approach that a highly precise solution can be acquired, even if it is a narrow count field.

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MEANS

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[Means for Solving the Problem] In order to attain the above-mentioned purpose, invention of claim 1 is characterized by including setting up so that it may permit that an impurity or a point defect moves to the boundary of the field which performs simulation across the boundary of a count field as boundary condition in the approach of performing the impurity or point defect diffusion simulation of a semiconductor production process.

[0010] Invention of claim 2 is characterized by the boundary condition in said claim 1 determining that the boundary condition of the boundary concerned will become equal to the movement magnitude obtained when it calculates in sufficient large field in which the movement magnitude of the impurity which passes through the boundary concerned, or a point defect includes the field concerned.

[0011] It is characterized by invention of claim 3 determining the boundary condition to which an impurity moves the boundary condition in said claim 1 across a boundary using the fine multiplier of the impurity profile of the direction [ / near the boundary ] of a boundary normal.

[0012] It is characterized by invention of claim 4 determining the boundary condition which an impurity or a point defect moves across a boundary when the boundary condition in said claim 1 approximates the impurity or point defect profile of the direction of a boundary normal with a gauss function. [ / near the boundary ]

[0013]

[Embodiment of the Invention] Hereafter, the operation gestalt of the simulation approach concerning this invention is explained to a detail, referring to a drawing. In the following operation gestalten, in order to simplify explanation, it considers as the 1-dimensional impurity diffusion simulation in a silicon substrate.

[0014] In the simulation approach explained with the following operation gestalten, the usual computer system equipped with output units, such as CPU for performing various processings, input devices, such as a keyboard, a mouse, a light pen, or flexible disk equipment, external storage, such as a memory apparatus and a disk unit, and a display unit, printer equipment, etc. is used. In addition, said CPU possesses the operation part which performs processing of each step explained below etc., and the primary storage which memorizes an instruction of said processing.

[0015] Gestalt drawing 1 of the 1st operation is a flow chart which shows processing actuation of the impurity diffusion simulation of this operation gestalt. Initiation of diffusion simulation sets the diffusion time of day T to 0 first (step S101). And the diffusion coefficient in diffusion temperature, a segregation coefficient, etc. are calculated, and a diffusion equation is set up (step S102).

[0016] Next, boundary condition is set up on the boundary of a simulation field, i.e., this example, as follows to a substrate base (step S103).

[0017]  $F = -D$  and  $\frac{dC}{dx}$  -- here, D is the diffusion coefficient of an impurity and C is high impurity concentration. This boundary condition means that an impurity flows out of a substrate base outside a simulation field by Flux F. The conventional approach had set up reflective mold conditions ( $F = 0$ ) as boundary condition here. For this reason, the impurity distribution which should spread by diffusion will be shut up for the reflective mold boundary condition set as the base, and concentration becomes high unusually. Although this problem was avoidable when setting up the simulation field sufficiently widely, the problem that computation time became long had arisen.

[0018] Thus, after setting up a diffusion equation and boundary condition, the solution to is calculated

using a numerical solution (step S104). Next, the increment of the diffusion time of day T in  $\Delta T$  is done (step S105), if it judges and (step S106) is not over whether the value is over all the diffusion time  $T_f$ , the loop formation which begins from a setup of the diffusion equation of step S102 is executed again, otherwise, count is ended.

[0019] Next, single diffusion simulation of the boron in a silicon substrate is made into an example, and the effectiveness of this invention is explained. Drawing 2 is 100keV(s) and  $3 \times 10^{13}/\text{cm}^2$  of doses about boron to a silicon substrate. It is a graph at the time of carrying out an ion implantation. The axis of abscissa of this graph shows the depth from a silicon substrate surface, and an axis of ordinate shows the concentration of boron. In order to simplify explanation, the impurity evaporation from a substrate front face was calculated as what is not. Here, it is spread at 1200 degrees C for 4 hours, and the result of having taken the sufficiently deep depth of a substrate with 8 micrometers, and having calculated it with a sufficient precision is shown in a broken line B. Moreover, an alternate long and short dash line C is the result of restricting the depth of a substrate to 2 micrometers and calculating using the conventional approach. By the conventional approach, since reflective mold boundary condition is used as boundary condition at the base of a substrate, boron will be shut up in a count field and has overestimated boron concentration remarkably. A continuous line shows the result which restricted the depth of a substrate to 2 micrometers and was calculated on the other hand using this invention.

[0020] The result depended on the simulation approach concerning this invention is shown in a thick wire D. Since the boundary condition of a simulation boundary was appropriately given like illustration, in spite of having restricted the simulation field to 2 micrometers, it is very well in agreement with the result (broken line B) calculated with a sufficient precision in the sufficiently large field. The impurity distribution near a substrate front face influences a component property greatly. Like drawing 2, since this invention calculates the impurity distribution near a substrate front face with a sufficient precision, the component property that precision is high can be acquired.

[0021] Thus, if this invention is used, simulation can be performed, without losing most precision, even if it narrows a simulation field. Although simulation fields were reduced to the quadrant in this example, it cannot be overemphasized that comparable reduction also of the amount of memory and computation time required for simulation is carried out. Thus, a process simulation can be performed at a high speed in the amount of memory smaller than before by using this invention.

[0022] In addition, although this operation gestalt explained using 1-dimensional simulation in order to simplify explanation, it is clear that this invention is applicable to two-dimensional and three-dimension simulation. It is clear that the amount of memory and the reduction effectiveness of computation time are especially remarkable in two-dimensional and three-dimension simulation.

[0023] What is necessary is just to set up boundary condition with the operation gestalt of the gestalt 1st of the 2nd operation, so that the solution near the solution calculated in the larger field may be acquired although boundary condition was calculated using the differential of impurity distribution by setup of the boundary condition of step S103. Therefore, it sets in this operation gestalt and, in the case of 1-dimensional simulation, is the profile of the direction of a boundary normal of the impurity distribution near the boundary, for example Gauss function  $a \cdot \exp[-b(x-x_0)^2]$

It comes out and approximates.  $x$  expresses the depth from a substrate front face here, and it is  $a$ ,  $b$ , and  $x_0$ . It is a constant. A gauss function becomes a solution to, when a diffusion coefficient is a constant as known well. Therefore, the impurity distribution near the base of a simulation field can be approximated with a sufficient precision with a gauss function. And the flux in a boundary is calculated noting that this gauss function is prolonged outside the field across the simulation boundary, and this value is used as boundary condition. Thus, since numerical differentiation will not be used like the above-mentioned operation gestalt if boundary condition is calculated, count which was not dependent on mesh spacing etc. and was stabilized can be performed. Consequently, a more accurate simulation result than the conventional approach is obtained.

[0024] Although the operation gestalt of the gestalt above of the 3rd operation explained diffusion of the impurity in a silicon substrate, it is also applicable to the diffusion simulation of a point defect and an impurity. Since impurity diffusion is influenced of a point defect, it can describe impurity diffusion with a precision more sufficient [ the diffusion equation which adopted the point defect ] than an impurity independent diffusion equation.

[0025] however, since the diffusion rate was alike and quicker than the impurity, the point defect needed to make the simulation field large very much, when the conventional approach was used. For example, in a substrate front face to a depth of about 10 micrometers, although a count field is good, when a point defect is adopted, it is [ about 100 micrometers of depth numbers ] needed [ with the process simulation of the usual MOSFET / field ]. For this reason, computation time was very long when a lot of memory was needed, in order to carry out simulation which took in point defect diffusion.

[0026] However, a count field required for impurity independent diffusion is set up, for example, and boundary condition is applied to a point defect by the approach used to the impurity with the 1st operation gestalt. If it does in this way, also in a narrow field comparable as the case where only impurity diffusion is dealt with, simulation becomes possible and the amount of memory requirements and computation time can be reduced sharply.

[0027] If the operation gestalt of these simulation approach is used as explained above, the process simulation of a semiconductor device can be limited to a required field, and can be performed. Therefore, it becomes possible in the amount of memory smaller than before to perform simulation at a high speed. Moreover, although there was a case where the precision of the count result obtained when the simulation field was narrow got very bad, by the conventional approach, since the fall of count precision is controlled even if a simulation field is narrow, if this invention is used, possibility of being confused by the inaccurate count result can be reduced.

[0028] If boundary condition is calculated using the differential of the impurity profile of the direction of a boundary normal as the 1st operation gestalt explained, the effectiveness of this invention is realizable only by repairing a little conventional program. Moreover, it is so short that computation time required for count of boundary condition can almost be disregarded if it is compared with the computation time which simulation takes.

[0029] Moreover, as the 2nd operation gestalt explained, boundary condition approximates the direction profile of a boundary normal of the impurity distribution near the boundary with a gauss function, it calculates the flux in a boundary, assuming that this function is prolonged outside a boundary, and sets up boundary condition using this. Since boundary condition can be set up without using numerical differentiation if it does in this way, the boundary condition for which it is hard to depend on the mesh used for numerical calculation can be set up.

[0030] Furthermore, as the 3rd operation gestalt explained, it is applicable not only to impurity diffusion but the diffusion simulation of a point defect and an impurity. the diffusion rate of an impurity boiled the point defect markedly, and since it was quick, when the conventional approach was used, it needed to make the simulation field large very much. For this reason, in order to carry out simulation which took in point defect diffusion, a lot of memory was needed, and computation time was very long. However, if this invention is applied, also in a narrow field, simulation becomes possible and the amount of memory requirements and computation time can be reduced sharply.

[0031] In addition, the program for realizing the simulation approach mentioned above can be saved at a record medium. This record medium can be made to be able to read according to a computer system, and the simulation approach mentioned above while executing said program and controlling the computer can be realized. Here, with said record medium, equipments which can record a program, such as a memory apparatus, a magnetic disk drive, and an optical disk unit, are contained.

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[Translation done.]

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DESCRIPTION OF DRAWINGS

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[Brief Description of the Drawings]

[Drawing 1] It is the flow chart which shows processing of the operation gestalt of the simulation approach concerning this invention.

[Drawing 2] It is the graph showing the well impurity distribution at the time of performing a process simulation by the simulation approach of this operation gestalt. An axis of abscissa shows the depth from a substrate front face, and an axis of ordinate shows boron concentration.

[Drawing 3] It is the graph showing impurity distribution of the well at the time of using the conventional process-simulation approach. An axis of abscissa shows the depth from a substrate front face, and an axis of ordinate shows boron concentration.

[Description of Notations]

A Boron concentration distribution immediately after an ion implantation

B Boron concentration distribution at the time of calculating to a depth of 8 micrometers

C Boron concentration distribution at the time of calculating to a depth of 2 micrometers

D Boron concentration distribution at the time of calculating to a depth of 2 micrometers using the simulation approach of this operation gestalt

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[Translation done.]

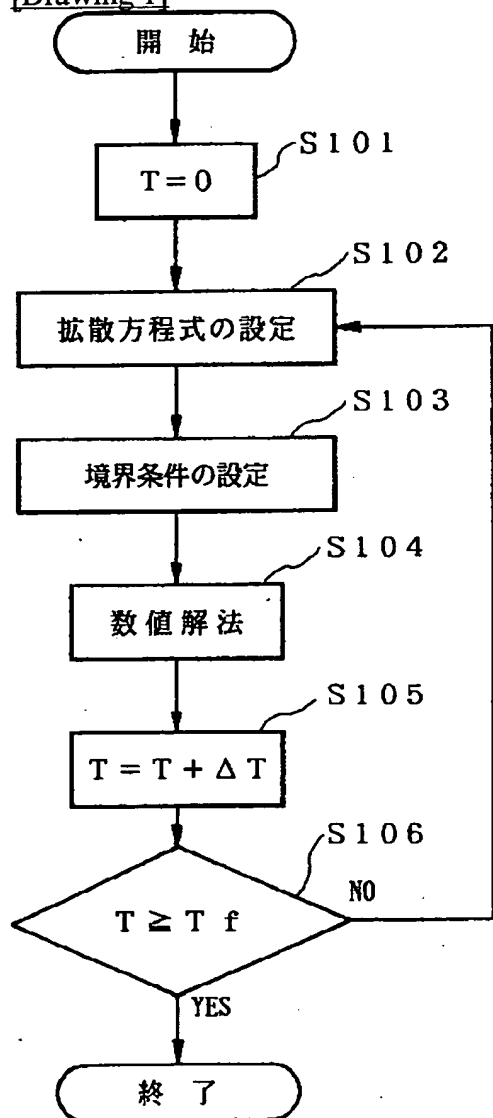
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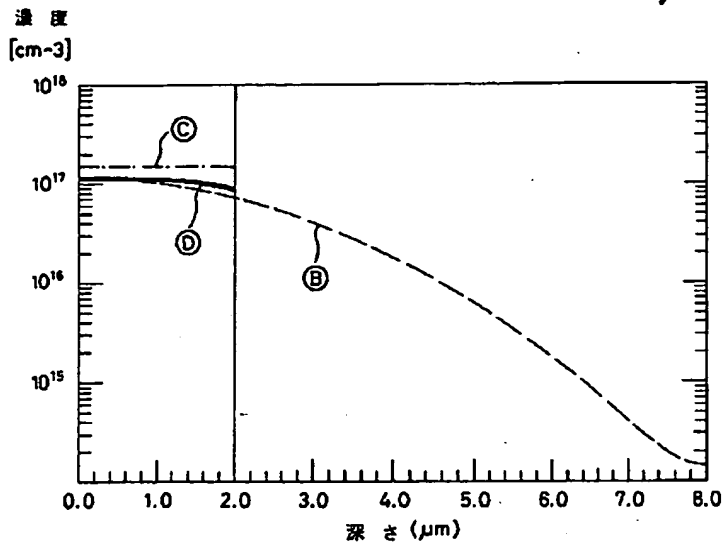
## DRAWINGS

[Drawing 1]

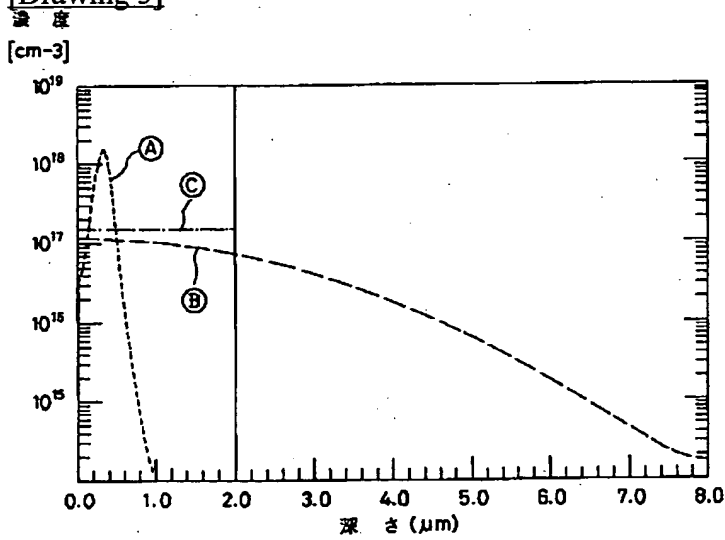


[Drawing 2]





[Drawing 3]



[Translation done.]